

# The Effect of Cr Concentration on Defect Energies in FeCr Alloys



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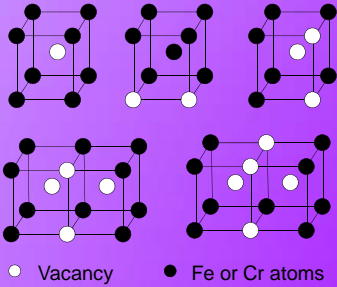
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**Abstract:** FeCr ferritic alloys are leading candidates for structural applications in generation IV fission reactors due to their high resistance to swelling and corrosion. The addition of Cr improves the behavior of the steels under irradiation, but this improvement is non-monotonic. Understanding the changes in the FeCr ferritic alloys microstructure induced by irradiation and the role played by the alloying element (Cr) is needed in order to predict the response of these materials under the extreme conditions in the future nuclear plants. In this work, we present the effect of Cr concentration in a bcc Fe matrix on binding and formation energies of vacancy clusters.

**Method:** Molecular static calculations with two different interatomic empirical potentials specially developed for the study of FeCr alloys have been performed in the study of the formation and binding energies of the vacancy clusters. One potential is based on a two-band model formalism (2BM)<sup>1</sup> and the other one has been created introducing an explicit dependence on concentration (CDM)<sup>2</sup>. Initial calculations in order to determine the cluster geometry more stable for each cluster size (up to 5) have been performed over size cells of 2000 atoms. Calculations for the more stable geometries of each cluster size and exploring all the possibilities of the cluster environment were performed on size cells of 250 atoms.

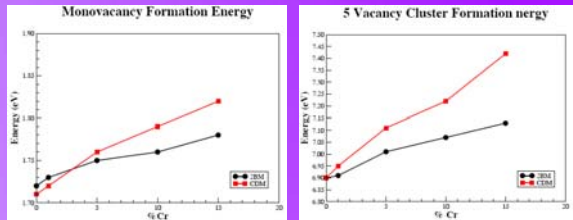
## Results and Discussion



### More stable configurations for vacancy clusters

- Only 1nn taken into account except in the case of the divacancy, where the 2nn vacancy cluster is more stable than the 1nn vacancy cluster.

### Vacancy cluster formation energy (mean value from the above histograms)



$$E_f = E_{\text{defect}} - (E_{\text{without defect}} - n_{\text{Fe}} E_{\text{Fe}} - n_{\text{Cr}} E_{\text{Cr}} - \Delta h)$$

$E_f$  = Formation energy of the defect

$E_{\text{defect}}$  = Energy of the cell with a defect

$E_{\text{without defect}}$  = Energy of the cell without a defect

$n_{\text{Fe}}$ ,  $n_{\text{Cr}}$  = Number of Fe or Cr atoms removed, respectively

$E_{\text{Fe}}$  = Energy of the Fe perfect cell per atom

$E_{\text{Cr}}$  = Energy of the Cr perfect cell per atom

$\Delta h$  = Enthalpy difference between initial and final % Cr

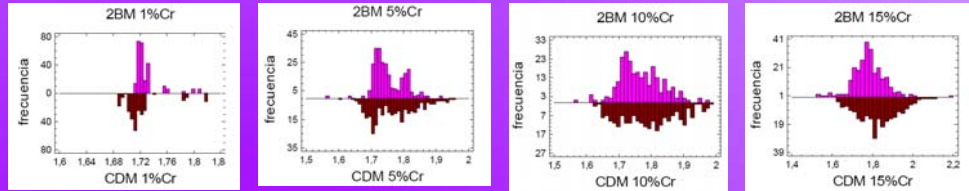
- Formation energy increases with:
  - The cluster size
  - The Cr concentration

- CDM potential predicts higher formation energies than the 2BM potential.
- These differences are greater for higher Cr concentrations

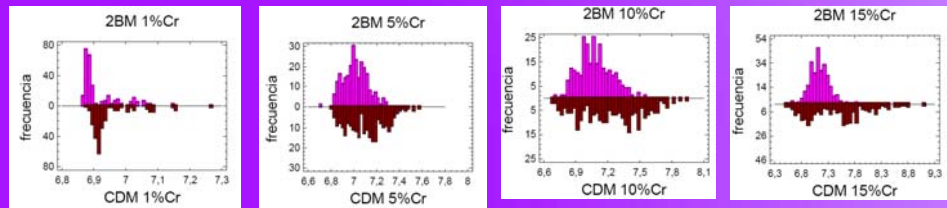
## Conclusions

- CDM potential more sensitive to the Cr local concentration
- Similar results for the vacancy cluster formation energy for both potentials studied
- Differences in the formation energy between CDM and 2BM potentials more appreciable with:
  - the Cr concentration
  - the size of the cluster
- Stability increases with the cluster size for vacancy clusters up to 5
- Binding energy does not depend on the Cr concentration for both potentials.

### Monovacancy



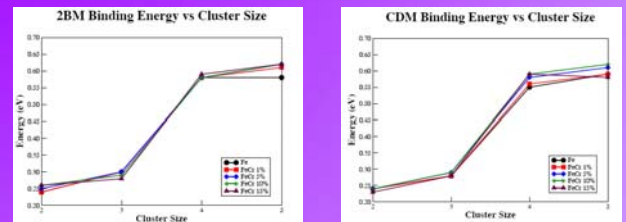
### 5 Vacancy Cluster



### Vacancy cluster formation energy histograms for 1 and 5 vacancies and 1,5,10,15 % Cr for the two interatomic potentials (top 2BM, bottom CDM)

- Higher Cr concentrations or cluster size provide more possibilities of having Cr at 1nn or 2nn positions  $\Rightarrow$  Greater dispersion of values in the formation energy between different configurations for the same cluster size and Cr concentration.
- Higher dispersion for the CDM potential.

### Binding energy of a single vacancy to a cluster of size n (n from 2 to 5 defects)



$$E_{a-b} = E_a + E_b - E_{ab}$$

$E_{a-b}$  = Binding energy between defect b and 1 vacancy

$E_a$  = Monovacancy formation energy

$E_b$  = (n-1) Vacancy cluster formation energy

$E_{ab}$  = n Vacancy cluster formation energy

- Similar energies with CDM and 2BM potentials
- Same energy values for Fe or FeCr alloys with 1,5,10,15% Cr
- Energy increases with the cluster size
- Small increases in the binding energy for 3 and 5 vacancy clusters with respect to the 2 and 4 vacancy clusters respectively
- Great increase in the binding energy for 4 vacancy clusters from 3 vacancy clusters

## Further work

- Study the effect of the Cr concentration on:
  - 111, 110 and 100 FeFe and FeCr Interstitials Formation Energy
  - Formation and Binding energies of Interstitial Clusters
- Study the effect of the Cr local concentration on the Interstitial Formation Energies
- Study the mobility of the interstitial in the FeCr alloy

## References

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c - E. del Río, J. M. Sampedro, H. Dogo, M. J. Caturla, M. Caro, A. Caro and J. M. Perlado. J. Nucl. Mater. (2010), doi: 10.1016/j.nucmat.2010.10.021

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